Study on nonmagnetic impurities in the superconducting state of two-dimensional t-J model

Hideki Tanaka[a], Kazuhiro Kuboki[a] and Manfred Sigrist[b]

[a] *Department of Physics, Kobe University, Kobe 657-8501, Japan*
[b] *Yukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-8502, Japan*

We study the effect of nonmagnetic impurities in the superconducting state of the $t - J$ model. The Bogoliubov de Gennes equation is derived using a slave-boson mean-field approximation, and we solve it numerically at $T = 0$. The $d_{x^2-y^2}$-wave order parameter is suppressed near an impurity and its spatial variation induces the extended s-wave component. We also find the local charge density wave (CDW)-like feature due to the Friedel oscillations. This leads to the splitting of the expected zero-energy Andreev bound state. Therefore the system is unlikely introducing a localized state of other symmetry such as superconductivity with broken time reversal symmetry or antiferromagnetism.

The symmetry of the superconducting (SC) state in high-T_c superconductors (HTSC) has been a subject of intensive study since it is an important clue to clarify the mechanism of their superconductivity.[1] Now it is established that the SC state has a predominantly $d_{x^2-y^2}$-wave character with a possible mixture of an s-wave component due to the orthorhombic lattice distortion in some systems. In d-wave superconductors the effect of nonmagnetic impurities is quite different from that of conventional (s-wave) superconductors because of the phase structure of the pair wavefunction and the resulting presence of nodes in the excitation gap. This problem has been studied intensively by many authors, mostly based on weak coupling theories.[2, 3, 4, 5, 6] In this letter we examine the effect of nonmagnetic impurities in the SC state of the t-J model on a square lattice. This model describes the low-energy electronic properties of HTSC[7, 8] where strong correlation effects for the electrons are known to be important. Mean-field (MF) theories based on a slave-boson method predict a superconducting state with a $d_{x^2-y^2}$-symmetry.[9, 10] They may also explain the magnetic[11, 12] as well as the transport[13] properties of HTSC if the gauge fields representing the fluctuations around the MF solutions are taken into account. Therefore the effect of nonmagnetic impurities in the SC states of the t-J model is of particular interest.[14, 15]

We treat the t-J model with the Hamiltonian including that of the nonmagnetic impurities

$$H = \begin{aligned} &-t \sum_{<i,j>\sigma} (\tilde{c}_{i,\sigma}^{\dagger}\tilde{c}_{j,\sigma} + h.c.) \\ &+ J \sum_{<i,j>} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + V_0 \sum_{l\sigma} \tilde{c}_{l,\sigma}^{\dagger}\tilde{c}_{l,\sigma} \end{aligned} \tag{1}$$

where $\langle i, j \rangle$ and l denote nearest-neighbor bonds and the impurity sites, respectively, and $\tilde{c}_{i\sigma}$ is an electron operator within the Hilbert space excluding double occupancy. Here $\boldsymbol{S}_i$ is the spin-1/2 operator at a site i and $J(> 0)$

is the antiferromagnetic superexchange interaction. The impurity potential V_0 is taken to be $V_0 \gg J$. We use the slave-boson method to enforce the condition of no double occupancy by introducing spinons ($f_{i\sigma}$; fermion) and holons (b_i; boson) ($\tilde{c}_{i\sigma} = b_i^{\dagger}f_{i\sigma}$). We decouple this Hamiltonian by a mean-field approximation (MFA). In the following we consider only the case of $T = 0$, so that holons are Bose condensed. Then the mean-field Hamiltonian is written in terms of spinons only,

$$\mathcal{H}_{MFA} = \sum_i \sum_j [f_{i\uparrow}^{\dagger}, f_{i\downarrow}] \begin{bmatrix} W_{ij} & F_{ij} \\ F_{ji}^* & -W_{ji} \end{bmatrix} \begin{bmatrix} f_{j\uparrow} \\ f_{j\downarrow}^{\dagger} \end{bmatrix} \tag{2}$$

with

$$\begin{aligned} W_{ij} = & -\left(t\delta + \frac{3}{4}J\chi_{ij}\right)\sum_{\mu} \delta_{j,i+\mu} - \lambda\delta_{ij} + V_0\delta_{il}\delta_{jl} \\ F_{ij} = & -\frac{3}{4}J\Delta_{ij}\sum_{\mu}\delta_{j,i+\mu} \end{aligned} \tag{3}$$

where δ and λ are the doping rate and the chemical potential, respectively, and $\mu = \pm\hat{x}, \pm\hat{y}$. The summations for i and j are taken over all sites. Here the singlet RVB order parameter (OP), Δ_{ij}, and the bond OP, χ_{ij}, are defined as

$$\Delta_{ij} = \langle f_{i\downarrow}f_{j\uparrow} - f_{i\uparrow}f_{j\downarrow}\rangle/2, \quad \chi_{ij} = \sum_{\sigma}\langle f_{i\sigma}^{\dagger}f_{j\sigma}\rangle \tag{4}$$

respectively, for each nearest neighbor bond. We consider the solution where Δ_{ij} may be complex, while χ_{ij} is taken to be real (i.e., $\chi_{ij} = \chi_{ji}$). We do not consider the possible antiferrromagnetic correlation here.

Without impurities $\mathcal{H}_{MFA}$ can be easily diagonalized by the Bogoliubov transformation assuming spatially uniform χ and Δ. In the presence of inhomogeneities, however, we have to take their spatial variations into account. They are most conveniently described by the Bogoliubov de Gennes (BdG) equation.[16] From eq.(2)

it is obtained as

$$\epsilon_n \left[\begin{array}{c} u_n(i) \\ v_n(i) \end{array} \right] = \sum_j \left[\begin{array}{cc} W_{ij} & F_{ij} \\ F_{ji}^* & -W_{ji} \end{array} \right] \left[\begin{array}{c} u_n(j) \\ v_n(j) \end{array} \right]. \quad (5)$$

Here $(u_n(i), v_n(i))$ is the wave function at a site i, and ϵ_n is the corresponding energy eigenvalue. The OP's χ_{ij} and Δ_{ij}, and the doping rate δ (we take λ as an input parameter) are expressed in terms of $u_n(i)$ and $v_n(i)$,

$$\chi_{ij} = 2 \sum_n \left[u_n^*(i) u_n(j) f(\epsilon_n) + v_n(i) v_n^*(j) \{1 - f(\epsilon_n)\} \right]$$

$$\Delta_{ij} = \frac{1}{2} \sum_n \left[\{v_n^*(i) u_n(j) + v_n^*(j) u_n(i)\} f(\epsilon_n) \right. \\ \left. - \{u_n(i) v_n^*(j) + u_n(j) v_n^*(i)\} \{1 - f(\epsilon_n)\} \right]$$

$$\delta = 1 - \frac{2}{N} \sum_n \sum_i \left[|u_n(i)|^2 f(\epsilon_n) \right. \\ \left. + |v_n(i)|^2 \{1 - f(\epsilon_n)\} \right]$$

$$(6)$$

where $f(\epsilon)$ is the Fermi distribution function and N is the total number of lattice sites.

We numerically solve the self-consistency equations (5) and (6). For simplicity we assume that χ_{ij} has a spatially uniform value (obtained by MFA without impurity) except for the bonds connected to the impurity sites where $\chi_{ij} = 0$. First we choose λ, and assume some initial values of Δ_{ij} and δ. Inserting these into the BdG equation we diagonalize the resulting matrix using Householder method (the size of the matrix is $2M^2 \times 2M^2 (= 2N \times 2N)$, if the system size is $M \times M (= N)$).[17] Then we recalculate Δ_{ij} and δ according to eq.(6). This procedure is iterated until the convergence is reached. From Δ_{ij} we define a $d_{x^2-y^2}$- and an extended s- wave OP component on the site i,

$$\Delta_d(i) \equiv (\Delta_{i,i+x} + \Delta_{i,i-x} - \Delta_{i,i+y} - \Delta_{i,i-y})/4 \\ \Delta_s(i) \equiv (\Delta_{i,i+x} + \Delta_{i,i-x} + \Delta_{i,i+y} + \Delta_{i,i-y})/4, \quad (7)$$

where x and y correspond to one lattice constant in x- and y-direction, respectively. We have checked that the values obtained for the system without impurities agree well with those in the usual mean-field calculation, when $M \geq 16$. In this case only Δ_d is finite and it has a spatially uniform value.

Now we turn to the results for the system with an impurity. We consider the case where the concentration of impurities is low so that the states around the impurities can be treated independently. We fix $t/J = 3$ throughout in the following, and the doping rates are chosen to be $\delta = 0.20$. (We have studied the system with $0.05 \leq \delta \leq 0.20$. The results are qualitatively the same for all cases.) In Fig.1 the spatial variation of Δ_d is shown, which is suppressed near the impurity, and the effect is strongest along the diagonals of the square lattice. This is due to the interference effects for momenta close to the gap nodes (sign change of the pair wave function). The extended s-wave component is induced in the region where Δ_d is not uniform (Fig.2), and Δ_s at sites rotated 90 degree around the impurity have the same magnitude but the opposite sign. It vanishes for sites located along the diagonals passing through the impurity site. (Δ_d and

Δ_s are always real in the solutions we found.)

We analyze the above results qualitatively by using the GL theory (though GL theory is not quantitatively valid at $T = 0$). The GL free energy for the system with an impurity is written generically as[18]

$$\mathcal{F} = \int d^2 \boldsymbol{r} \Big[\sum_{j=d,s} \{\tilde{a}_j(T)|\Delta_j|^2 + \beta_d|\Delta_j|^4 + K_j|\boldsymbol{\nabla}\Delta_j|^2\} \\ + \gamma_1|\Delta_d|^2|\Delta_s|^2 + \tfrac{1}{2}\gamma_2(\Delta_d^{*2}\Delta_s^2 + \Delta_d^2\Delta_s^{*2}) \\ + \tilde{K}\{(\partial_x\Delta_d)^*(\partial_x\Delta_s) - (\partial_y\Delta_d)^*(\partial_y\Delta_s) + c.c\} \\ + g_d\delta(\boldsymbol{r})|\Delta_d|^2 + g_s\delta(\boldsymbol{r})|\Delta_s|^2 \Big]$$

$$(8)$$

where the last line represents the effect of the impurity located at $\boldsymbol{r} = 0$ ($g_d > 0$, $g_s > 0$), and the crystal axis directions are denoted as x and y. We note that the coupling term like $(\Delta_d\Delta_s^* + c.c.)$ should not arise due to the symmetry. Due to the g_d term Δ_d is suppressed and its gradient becomes finite over the range of the coherence length. Then Δ_s is induced through the mixed gradient ($\tilde{K}$)-term. In the $\tilde{K}$-term the gradients in x and y directions have opposite sign following the Δ_d-symmetry, and the induced Δ_s must reflect this property. Therefore Δ_s should change sign under 90-degree rotation around the impurity. When the continuous change of the phases of Δ_d and Δ_s were allowed, Δ_s could change sign under 90-degree rotation with keeping its amplitude finite (i.e., $\phi_{ds} = \pm\pi/2$ along the diagonals). If the relative phase between Δ_d and Δ_s (ϕ_{ds}) is neither 0 or π, the state has $(d+is)$- or $(d-is)$-symmetry and breaks time reversal symmetry $\mathcal{T}$.[19,20] In this case the gap nodes disappear in the vicinity of the impurity and the system could gain more condensation energy. In our calculation no solution of this type with Δ_d and Δ_s in a complex combination appeared for the doping range $0.05 \leq \delta \leq 0.20$. In the following we would like to discuss a possible reason for this result.

It has been discussed previously based on the T-matrix approximation that non-magnetic impurities in a d-wave superconductor create a subgap bound state,[5] similar to Shiba's bound state in a conventional superconductor around a magnetic impurity.[21] In the T-matrix formulation it is found that a single bound state occurs at the Fermi level (zero-energy) in the unitary limit, i.e. for a strong impurity potential.[5] This is understood also within the BdG formulation as an Andreev bound state.[22] Because a strong scattering center destroys the gap in the near vicinity of the impurity, quasiparticles can be trapped in this potential well and is subject to Andreev reflection at the walls of this well. Their energies are determined by the phase of the gap function in the momentum directions which the particle-hole trajectories connect via scattering at the impurity.[22] For the d-wave superconductor there are two possible phase differences, 0 and π. The former leads to a state at the bulk gap value while the later generates a zero-energy bound state similar to the one at the [110]-oriented surface of a $d_{x^2-y^2}$-wave superconductor.[22,23,24,25,26,27,28] The presence of the latter bound states should yield a

finite contribution of local density of states (LDOS) at the Fermi energy. In this case it could be energetically favorable to twist the OP phase in order to shift the zero-energy bound state away from the Fermi energy. Such a state would then correspond to the state with locally broken time reversal symmetry around the impurity as mentioned above. This effect is, of course, a matter of competition between the energy gain of the quasiparticles and the energy expense due to phase gradients (yielding supercurrents) introduced by the twist.

In order to examine this view we consider the LDOS which is denoted as $N(\boldsymbol{r}_i, \omega)$ on the site i,

$$N(\boldsymbol{r}_i, \omega) = \sum_n \left[|u_n(i)|^2 \delta(\omega - \epsilon_n) + |v_n(i)|^2 \delta(\omega + \epsilon_n) \right]. \tag{9}$$

In Fig.3 we show the result for $N(\boldsymbol{r}_i, \omega)$ for a nearest neighbor site of the impurity ($\delta = 0.20$). At an energy much lower than the gap value ($\Delta_d \sim 0.12$) we find bound states. The bound state energy is different from the naively expected value, i.e., zero, leading to a small gap between the state below and above the Fermi energy. The LDOS is different for these two states, since the doped system is not particle-hole symmetric.

The splitting of the expected zero-energy bound state into levels slightly above and below zero occurs obviously without the $\mathcal{T}$-violation, since our solution has only real superconducting OP's. This splitting may have various reasons. The validity of arguments based on the Andreev approximation might not be guaranteed here. Another important aspect is, however, connected with charge density oscillations as shown in Fig.4. They originate from the Friedel oscillations due to the presence of the impurity. The dominant Q-vector lies along the [110]-direction which is for $\delta = 0.2$ very close to $\mathbf{Q} = (\pi, \pi)$ and leads to a nearly commensurate charge density staggering. In the vicinity of the impurity these lead to a charge density wave (CDW) like environment with an effective "doubling of the unit cell" so that the local opening of a gap is expected. We would like to emphasize, however, that this CDW feature is not the result of an instability triggered by the quasiparticle density of states at the Fermi level, but is driven by the presence of the impurity. The fact that there is no quasiparticle peak in the LDOS at zero energy leads to the conclusion that a transition to a state with local $\mathcal{T}$-violation or antiferromagnetic order is very unlikely to occur.

In summary we have studied the effects of nonmagnetic impurities in the superconducting state of the t-J model using the Bogoliubov de Gennes equation derived via a slave-boson mean-field approximation. Near the impurity the d-wave OP is suppressed, and the extended s-wave component is induced as expected also from the GL description. The CDW-like feature due to the Friedel oscillations is most likely responsible for the double peak structure found in the LDOS at energies close to zero. We conclude that the violation of time reversal symmetry is suppressed here due to the removal of a quasiparticle bound state at zero energy. This is in contrast to the situation at the surface or at interfaces between d-wave superconductors.

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Fig. 1 The spatial variation of Δ_d in the system with an impurity. Here $\delta = 0.20$, $t/J = 3$ and the system size is $N = 16 \times 16$.

Fig. 2 The spatial variation of Δ_s in the system with an impurity. Here $\delta = 0.20$, $t/J = 3$ and the system size is $N = 16 \times 16$.

Fig. 3 LDOS at a nearest neighbor site of the impurity with $\delta = 0.20$, $t/J = 3$ and $N = 18 \times 18$. Here we have introduced finite width $\Gamma = 0.008J$ to each state.

Fig. 4 The electron density around the impurity. Here $\delta = 0.20$, $t/J = 3$ and the system size is $N = 18 \times 18$.

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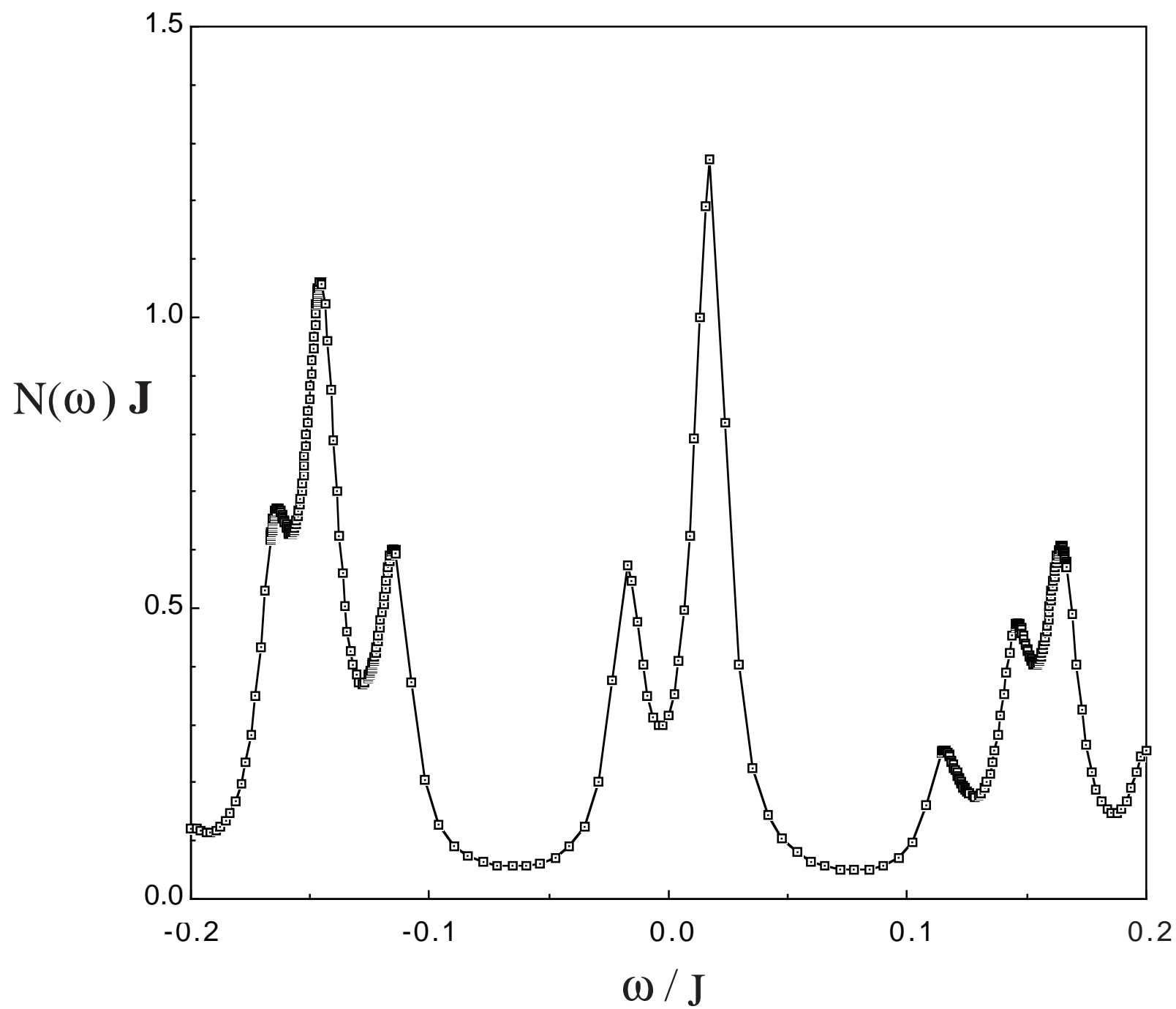
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Fig.3

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